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catena-Poly[cobalt(II)-bis(μ-3,7-dichloroquinoline-8-carboxylato-$\kappa^3N,O:O'$)]

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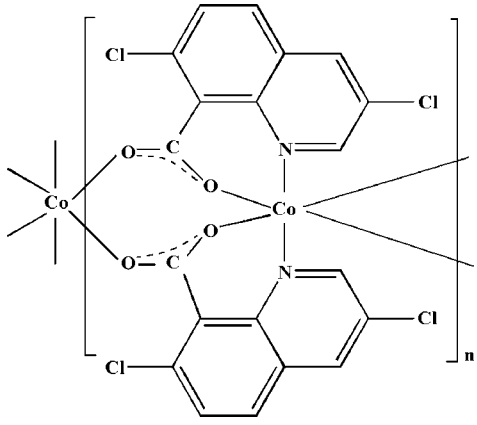
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.089; data-to-parameter ratio = 12.4.

In the crystal structure of the title compound, $[Co(C_{10}H_4Cl_2NO_2)_2]_n$, the Co^{II} cation lies on a twofold rotation axis. Each cation is *N*,*O*-chelated by the carboxylate anions of two 3,7-dichloroquinoline-8-carboxylate ligands. The second carboxylate O atom of each ligand coordinates to the Co^{II} cation of an adjacent molecule, linking the cations into a linear chain. Strong interchain π–π stacking interactions are observed in the crystal structure (perpendicular distance 3.42 Å, centroid-to-centroid distance 3.874 Å)

Related literature

For the use of 3,7-dichloro-8-quinolinecarboxylic acid as a herbicide, see: Nuria *et al.* (1997); Pornprom *et al.* (2006); Sunohara & Matsumoto (2004); Tresch & Grossmann (2002). For related vanadium and cadmium complexes, see Chen *et al.* (2001); Yang *et al.* (2005). For related literature, see: Turel *et al.* (2004); Zhang *et al.* (2007).



Experimental

Crystal data

$[Co(C_{10}H_4Cl_2NO_2)_2]$
M_r = 541.01
Orthorhombic, *Pccn*
a = 13.5109 (14) Å
b = 15.964 (2) Å
c = 9.2157 (16) Å
V = 1987.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 298 (2) K
0.49 × 0.33 × 0.31 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.57, T_{max} = 0.64
9558 measured reflections
1752 independent reflections
1404 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.11
1752 reflections
141 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.093 (2)	Co1—N1	2.197 (2)
Co1—O2^{i}	2.057 (2)		
O2^{i}—Co1—O2^{ii}	103.60 (12)	O2^{ii}—Co1—N1	87.24 (9)
O2^{i}—Co1—O1	170.96 (9)	O1—Co1—N1	89.82 (9)
O2^{ii}—Co1—O1	85.43 (8)	O1^{iii}—Co1—N1	92.31 (9)
O1—Co1—O1^{iii}	85.55 (12)	N1^{iii}—Co1—N1	177.10 (14)
O2^{i}—Co1—N1	90.97 (9)		

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+\frac{3}{2}, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2456).

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supplementary materials

Acta Cryst. (2008). E**64**, m227 [**doi:10.1107/S1600536807066755**]

catena-Poly[cobalt(II)-bis(μ-3,7-dichloroquinoline-8-carboxylato-$\kappa^3N,O:O'$)]

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Comment

Quinolinecarboxylates generally chelate to metal atoms, and some metal quinolinecarboxylates have been reported such as, for example, bis(6-methyl-4-hydroxy-3-quinolinecarboxylate) mono(oxo)monohydroxyvanadium(V) and $Cd(H_2O)(4\text{-quinolinecarboxylato})_2$ (Chen *et al.*, 2001; Yang *et al.*, 2005). Quinclorac (3,7-dichloro-8-quinolinecarboxylic acid) is a most effective herbicides (Nuria *et al.*, 1997; Pornprom *et al.*, 2006; Sunohara & Matsumoto, 2004; Tresch & Grossmann, 2002). We have reported a nickel-quinclorac complex in our previous work (Zhang *et al.*, 2007). The title compound is a cobalt(II) derivative (I) (Fig. 1) with the Co^{II} cation located on a twofold rotation axis. The Co^{II} center exhibits a distorted octahedral geometry defined by four carboxylato oxygen atoms from four quinclorac and two nitrogen atoms from two quinclorac units. Each quinclorac ligand chelates to the cobalt atom *via* a quinoline N atom and a carboxylate O atom. Adjacent molecules are linked by carboxylate bridges into a linear chain. The chains are assembled into a three-dimensional supramolecular architecture by strong offset face-to-face π–π stacking interactions (perpendicular distance: 3.42 Å, centroid-centroid distance: 3.874 Å) between the C2–C7 and $C2^i$–$C7^i$ benzene rings [symmetry code: (i) 2 - *x*, 1 - *y*, - *z*].

Experimental

A mixture of quinclorac (0.5 mmol, 0.121 g), $CoCl_2.6H_2O$ (1 mmol, 0.238 g), $Na_2MoO_4.2H_2O$ (0.5 mmol, 0.121 g) and H_2O (10 ml) was treated with aqueous HCl to a pH of 5. The mixture was placed in a Teflon-lined autoclave; this was heated at 403 K for three days. Red crystals were collected and washed with water. C H & N elemental analysis. Calculated for $C_{20}H_8Cl_4N_2O_4Co$: C 44.36, H 1.48, N 5.18%; found: C 44.48, H 1.69, N 5.31%. Selected FT—IR (KBr, cm^{-1}): 3301(w), 1581(*s*), 1553(*m*), 1482(*m*), 1402(*m*), 1383(*s*), 1232(*m*), 1139 (*m*), 1101(*s*), 761(*m*), 553(*m*), 449(*m*).

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

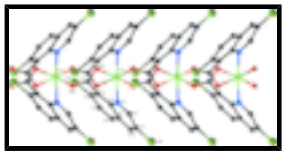

Fig. 1. The structure of (I), with the atomic numbering scheme and displacement ellipsoids at the 50% probability level. H atoms have been omitted for clarity [Symmetry code: (i) *x*,-*y* + 1/2,*z* + 1/2.]

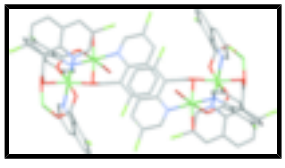

Fig. 2. Three dimensional supramolecular architecture constructed by interchain π–π stacking interactions.

catena-Poly[cobalt(II)-bis(μ-3,7-dichloroquinoline-8-carboxylato- $\kappa^3N,O:O^1$)] ?

Crystal data

$[Co(C_{10}H_4Cl_2NO_2)_2]$	F_{000} = 1076
	D_x = 1.808 Mg m^{-3}
M_r = 541.01	D_m = 1.800 Mg m^{-3}
	D_m measured by not measured
Orthorhombic, *Pccn*	Mo *K*α radiation
	λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 9558 reflections
a = 13.5109 (14) Å	θ = 2.0–25.0º
b = 15.964 (2) Å	μ = 1.43 mm^{-1}
c = 9.2157 (16) Å	*T* = 298 (2) K
V = 1987.7 (5) Å^3	Block, red
Z = 4	0.49 × 0.33 × 0.31 mm

Data collection

Siemens SMART CCD area-detector diffractometer	1752 independent reflections
Radiation source: fine-focus sealed tube	1404 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −16→13
T_{min} = 0.57, T_{max} = 0.64	*k* = −18→18
9558 measured reflections	*l* = −10→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.089	$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 3.6236P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max}$ = 0.001
1752 reflections	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
141 parameters	$\Delta\rho_{min}$ = −0.76 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.7500	0.7500	0.25905 (6)	0.02337 (17)
Cl1	0.77826 (7)	0.45967 (6)	−0.08682 (10)	0.0438 (3)
Cl2	1.11100 (8)	0.71113 (7)	0.54570 (14)	0.0641 (4)
N1	0.89374 (19)	0.68581 (16)	0.2651 (3)	0.0271 (6)
O1	0.70392 (16)	0.66997 (13)	0.0924 (2)	0.0296 (5)
O2	0.80139 (16)	0.65857 (13)	−0.1029 (2)	0.0287 (5)
C1	0.7764 (2)	0.64027 (19)	0.0240 (3)	0.0253 (7)
C2	0.8430 (2)	0.57762 (19)	0.0989 (3)	0.0254 (7)
C3	0.8519 (2)	0.4963 (2)	0.0541 (4)	0.0305 (7)
C4	0.9198 (3)	0.4403 (2)	0.1170 (4)	0.0406 (9)
H4	0.9214	0.3846	0.0871	0.049*
C5	0.9831 (3)	0.4674 (2)	0.2212 (4)	0.0405 (9)
H5	1.0300	0.4309	0.2594	0.049*
C6	0.9783 (2)	0.5510 (2)	0.2723 (4)	0.0325 (8)
C7	0.9051 (2)	0.60506 (19)	0.2140 (3)	0.0273 (7)
C8	0.9570 (2)	0.7133 (2)	0.3621 (4)	0.0325 (8)
H8	0.9503	0.7681	0.3949	0.039*
C9	1.0338 (2)	0.6646 (2)	0.4188 (4)	0.0378 (8)
C10	1.0438 (3)	0.5835 (2)	0.3773 (4)	0.0397 (9)
H10	1.0929	0.5499	0.4175	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0269 (3)	0.0247 (3)	0.0185 (3)	0.0027 (3)	0.000	0.000
Cl1	0.0472 (5)	0.0369 (5)	0.0472 (6)	−0.0042 (4)	−0.0028 (4)	−0.0106 (4)
Cl2	0.0561 (6)	0.0563 (7)	0.0799 (8)	0.0064 (5)	−0.0383 (6)	−0.0098 (6)
N1	0.0271 (14)	0.0274 (14)	0.0268 (15)	0.0037 (11)	−0.0010 (11)	0.0010 (11)
O1	0.0316 (12)	0.0338 (12)	0.0233 (12)	0.0062 (10)	−0.0014 (10)	−0.0035 (10)
O2	0.0344 (12)	0.0307 (12)	0.0211 (12)	0.0016 (10)	0.0015 (9)	0.0020 (10)
C1	0.0322 (17)	0.0217 (15)	0.0220 (16)	−0.0028 (12)	−0.0030 (13)	0.0000 (12)
C2	0.0258 (16)	0.0285 (16)	0.0218 (16)	0.0024 (13)	0.0053 (13)	0.0052 (13)

C3	0.0331 (17)	0.0261 (17)	0.0323 (18)	−0.0021 (14)	0.0046 (14)	0.0002 (14)
C4	0.051 (2)	0.0242 (18)	0.047 (2)	0.0059 (16)	0.0032 (19)	−0.0001 (16)
C5	0.042 (2)	0.0340 (19)	0.045 (2)	0.0122 (16)	−0.0004 (17)	0.0073 (17)
C6	0.0332 (18)	0.0330 (18)	0.0311 (19)	0.0051 (14)	0.0012 (14)	0.0049 (15)
C7	0.0266 (16)	0.0289 (17)	0.0264 (17)	0.0044 (13)	0.0070 (13)	0.0044 (14)
C8	0.0292 (17)	0.0315 (18)	0.037 (2)	0.0018 (14)	−0.0010 (15)	0.0008 (15)
C9	0.0306 (18)	0.042 (2)	0.041 (2)	0.0018 (15)	−0.0088 (16)	−0.0023 (17)
C10	0.0337 (19)	0.045 (2)	0.040 (2)	0.0106 (16)	−0.0065 (16)	0.0053 (18)

Geometric parameters (Å, °)

Co1—O1	2.093 (2)	C2—C3	1.368 (4)
Co1—O1^{i}	2.093 (2)	C2—C7	1.422 (4)
Co1—O2^{ii}	2.057 (2)	C3—C4	1.406 (5)
Co1—O2^{iii}	2.057 (2)	C4—C5	1.357 (5)
Co1—N1^{i}	2.197 (2)	C4—H4	0.9300
Co1—N1	2.197 (2)	C5—C6	1.416 (5)
Cl1—C3	1.738 (3)	C5—H5	0.9300
Cl2—C9	1.734 (4)	C6—C10	1.410 (5)
N1—C8	1.312 (4)	C6—C7	1.419 (4)
N1—C7	1.381 (4)	C8—C9	1.398 (5)
O1—C1	1.257 (4)	C8—H8	0.9300
O2—C1	1.252 (4)	C9—C10	1.358 (5)
O2—Co1^{iv}	2.057 (2)	C10—H10	0.9300
C1—C2	1.512 (4)		
O2^{ii}—Co1—O2^{iii}	103.60 (12)	C7—C2—C1	119.2 (3)
O2^{ii}—Co1—O1	170.96 (9)	C2—C3—C4	122.5 (3)
O2^{iii}—Co1—O1	85.43 (8)	C2—C3—Cl1	119.6 (3)
O2^{ii}—Co1—O1^{i}	85.43 (8)	C4—C3—Cl1	117.9 (3)
O2^{iii}—Co1—O1^{i}	170.96 (8)	C5—C4—C3	120.0 (3)
O1—Co1—O1^{i}	85.55 (12)	C5—C4—H4	120.0
O2^{ii}—Co1—N1^{i}	87.24 (9)	C3—C4—H4	120.0
O2^{iii}—Co1—N1^{i}	90.97 (9)	C4—C5—C6	120.5 (3)
O1—Co1—N1^{i}	92.31 (9)	C4—C5—H5	119.8
O1^{i}—Co1—N1^{i}	89.82 (9)	C6—C5—H5	119.8
O2^{ii}—Co1—N1	90.97 (9)	C10—C6—C5	123.1 (3)
O2^{iii}—Co1—N1	87.24 (9)	C10—C6—C7	118.3 (3)
O1—Co1—N1	89.82 (9)	C5—C6—C7	118.6 (3)
O1^{i}—Co1—N1	92.31 (9)	N1—C7—C6	121.1 (3)
N1^{i}—Co1—N1	177.10 (14)	N1—C7—C2	118.5 (3)
C8—N1—C7	118.2 (3)	C6—C7—C2	120.5 (3)
C8—N1—Co1	115.9 (2)	N1—C8—C9	123.5 (3)
C7—N1—Co1	121.7 (2)	N1—C8—H8	118.2
C1—O1—Co1	111.49 (19)	C9—C8—H8	118.2
C1—O2—Co1^{iv}	130.7 (2)	C10—C9—C8	119.9 (3)

O2—C1—O1	126.2 (3)	C10—C9—Cl2	122.6 (3)
O2—C1—C2	114.9 (3)	C8—C9—Cl2	117.4 (3)
O1—C1—C2	119.0 (3)	C9—C10—C6	118.8 (3)
C3—C2—C7	117.8 (3)	C9—C10—H10	120.6
C3—C2—C1	122.9 (3)	C6—C10—H10	120.6
$O2^{ii}$—Co1—N1—C8	9.9 (2)	Cl1—C3—C4—C5	176.0 (3)
$O2^{iii}$—Co1—N1—C8	−93.6 (2)	C3—C4—C5—C6	3.0 (5)
O1—Co1—N1—C8	−179.1 (2)	C4—C5—C6—C10	−178.1 (4)
$O1^{i}$—Co1—N1—C8	95.4 (2)	C4—C5—C6—C7	1.0 (5)
$O2^{ii}$—Co1—N1—C7	166.4 (2)	C8—N1—C7—C6	4.7 (4)
$O2^{iii}$—Co1—N1—C7	62.8 (2)	Co1—N1—C7—C6	−151.2 (2)
O1—Co1—N1—C7	−22.7 (2)	C8—N1—C7—C2	−174.0 (3)
$O1^{i}$—Co1—N1—C7	−108.2 (2)	Co1—N1—C7—C2	30.1 (4)
$O1^{i}$—Co1—O1—C1	68.44 (19)	C10—C6—C7—N1	−4.1 (5)
$N1^{i}$—Co1—O1—C1	158.1 (2)	C5—C6—C7—N1	176.6 (3)
N1—Co1—O1—C1	−23.9 (2)	C10—C6—C7—C2	174.5 (3)
$Co1^{iv}$—O2—C1—O1	8.1 (5)	C5—C6—C7—C2	−4.8 (5)
$Co1^{iv}$—O2—C1—C2	−170.54 (19)	C3—C2—C7—N1	−177.0 (3)
Co1—O1—C1—O2	−109.2 (3)	C1—C2—C7—N1	7.7 (4)
Co1—O1—C1—C2	69.4 (3)	C3—C2—C7—C6	4.4 (4)
O2—C1—C2—C3	−65.8 (4)	C1—C2—C7—C6	−170.9 (3)
O1—C1—C2—C3	115.4 (3)	C7—N1—C8—C9	−1.4 (5)
O2—C1—C2—C7	109.2 (3)	Co1—N1—C8—C9	155.8 (3)
O1—C1—C2—C7	−69.6 (4)	N1—C8—C9—C10	−2.3 (6)
C7—C2—C3—C4	−0.3 (5)	N1—C8—C9—Cl2	179.7 (3)
C1—C2—C3—C4	174.8 (3)	C8—C9—C10—C6	2.8 (6)
C7—C2—C3—Cl1	−179.7 (2)	Cl2—C9—C10—C6	−179.4 (3)
C1—C2—C3—Cl1	−4.6 (4)	C5—C6—C10—C9	179.5 (4)
C2—C3—C4—C5	−3.4 (5)	C7—C6—C10—C9	0.4 (5)

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, *z*; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*+3/2, *y*, *z*+1/2; (iv) *x*, −*y*+3/2, *z*−1/2.

Fig. 1

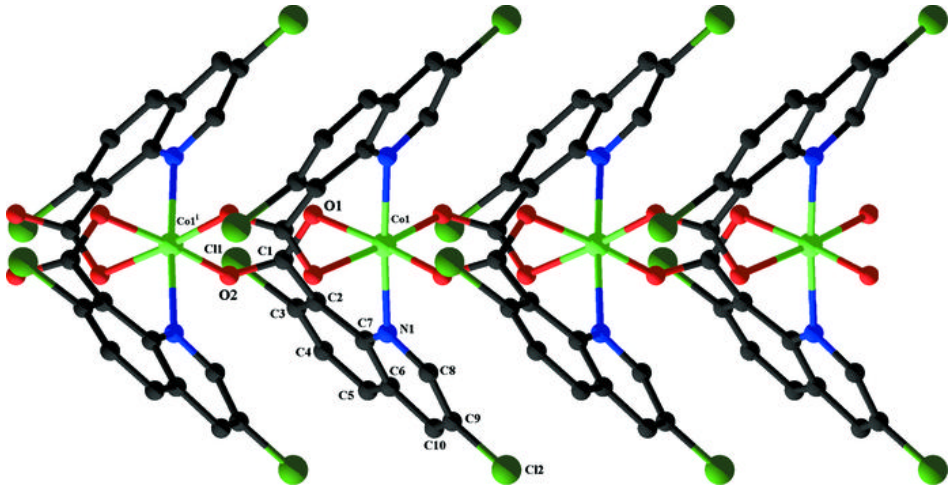

Fig. 2